Excitation of the Fe $^{\text{XIV}}$ spectrum in the Sun, stars and Seyfert galaxies: reconciling theory, observations and experiment

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Introduction

• Observational background
• Modelling Seyfert spectra
• Theoretical work on the Fe xiv $^2P^o_{1/2} - ^2P^o_{3/2}$ transition
• Current state of theory
• Latest theory compared to experiment
• Thermally averaged collision strengths
• Summary
Observational background

• Fe optical forbidden lines, including Fe XIV were identified by Gro-trian (1939) and Edlen (1943)
• Seen in the solar corona and in nova spectra in the 1930s
• In 1943 Seyfert identified several optical [Fe VII] lines in the spectra of the nuclei of some galaxies - to become known as Seyfert galaxies
• In the 1960s rocket borne spectrographs revealed the UV spectrum of the corona
• In 1968 Oke & Sargent report observations of a Seyfert Galaxy (NGC 4151) showing Fe XIV λ5303 and Fe X λ6374
• In the 1970s identifications of high ionization optical forbidden lines were also claimed in supernova remnants and binary stars
More recently Oliva et al (1994) obtained this optical and near infrared spectrum of a nearby (4Mpc) Seyfert, the Circinus galaxy (A1409-65)

The visible section clearly shows [Fe VII] $\lambda 6087$, [Fe X] $\lambda 6374$, [Fe XI] $\lambda 7892$ and [S VIII] $\lambda 9913$.
• while the near IR section clearly shows forbidden lines of Si vi $\lambda 1.963$, Si vii $\lambda 2.483$, Si ix $\lambda 3.935$, S ix $\lambda 1.252$ and Ca viii $\lambda 2.321$
Modelling Seyfert spectra

- The interest in Seyfert spectra here relates to the physical conditions in which the forbidden lines are formed.
- Oliva et al (1994) argue persuasively that the emitting gas is ionized by the hard UV continuum from the active galactic nucleus.
- They model the spectrum using a continuum with a double power law spectrum. Elemental abundances are assumed solar.
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<table>
<thead>
<tr>
<th>Ratio</th>
<th>Obs</th>
<th>Oliva et al (1994)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Fe x]/[S VIII]</td>
<td>2.4</td>
<td>3.2</td>
</tr>
<tr>
<td>[Fe xi]/[S VIII]</td>
<td>1.5</td>
<td>2.3</td>
</tr>
<tr>
<td>[Fe xiv]/[S VIII]</td>
<td>&lt;2.4</td>
<td>0.77</td>
</tr>
<tr>
<td>[Fe vii]/[S VIII]</td>
<td>1.3</td>
<td>1.4</td>
</tr>
<tr>
<td>[Si vi]/[S VIII]</td>
<td>2.0</td>
<td>1.6</td>
</tr>
<tr>
<td>[Si vii]/[S VIII]</td>
<td>3.2</td>
<td>2.2</td>
</tr>
<tr>
<td>[S ix]/[S VIII]</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>[Ca viii]/[S VIII]</td>
<td>1.5</td>
<td>0.59</td>
</tr>
</tbody>
</table>
Note that in these models the atomic parameters for Fe X, Fe XI and Fe XIV come from the distorted wave calculations of Mason (1975). The remainder are also the results of distorted wave calculations, mainly by Blaha (1968) and Krueger & Czyzak (1970). More sophisticated calculations using the close-coupling method were beginning to be made at this time as reported by Mason (1994) in her critical assessment of excitation data for Fe IX - Fe XIV. A year or two before this the Iron Project was set up and made its first goal the calculation of excitation data for ground state fine structure transitions - just those seen in the Seyfert galaxy spectra. Between 1994 and 1997, new collision strengths with a detailed treatment of resonances became available for all the ions in the above table except Fe VII and Fe IX.
Ferguson, Korista and Ferland (1997) made some general photoionization models of Seyfert galaxies using the new improved excitation rates.

They find that emission comes from gas at a few $\times 10^4$ K.

Their predictions are compared to the observations of the Circinus galaxy below.
• Ferguson, Korista and Ferland (1997) made some general photoionization models of Seyfert galaxies using the new improved excitation rates

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• Their predictions are compared to the observations of the Circinus galaxy below

<table>
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<tr>
<th>Ratio</th>
<th>Obs</th>
<th>Ferguson et al (1997)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Fe X]/[S VIII]</td>
<td>2.4</td>
<td>34.</td>
</tr>
<tr>
<td>[Fe XI]/[S VIII]</td>
<td>1.5</td>
<td>1.4</td>
</tr>
<tr>
<td>[Fe XIV]/[S VIII]</td>
<td>&lt;2.4</td>
<td>16.</td>
</tr>
<tr>
<td>[Fe VII]/[S VIII]</td>
<td>1.3</td>
<td>0.74</td>
</tr>
<tr>
<td>[Si VI]/[S VIII]</td>
<td>2.0</td>
<td>3.3</td>
</tr>
<tr>
<td>[Si VII]/[S VIII]</td>
<td>3.2</td>
<td>3.9</td>
</tr>
<tr>
<td>[S IX]/[S VIII]</td>
<td>1.0</td>
<td>5.0</td>
</tr>
<tr>
<td>[Ca VIII]/[S VIII]</td>
<td>1.5</td>
<td>5.3</td>
</tr>
</tbody>
</table>
• Agreement between the model predictions and theory is worse with some large differences
• The differences for Fe X and Fe XIV are particularly large
• Ferguson et al estimate that the abundance of Fe would have to be reduced by an order of magnitude relative to other elements to get agreement for these ions
• There is no physical reason to expect such a result and they question the accuracy of the calculated excitation cross-sections
Theoretical work on the Fe XIV $^{2}P_{1/2}^{0} - ^{2}P_{3/2}^{0}$ transition

- How accurate are the near threshold excitation data (collision strengths) for these ions?

- The collision strengths used by Ferguson *et al* for direct excitation of the $\lambda 5303$ transition is from Storey, Mason and Saraph (1996)
Current state of theory

- Two new and very elaborate calculations of collision strengths for Fe$^{13+}$ exist
- Tayal, (ApJS, 178, 359, 2008) use the Breit-Pauli R-matrix approach in a 135-level calculation, including some n=4 states
- Liang et al (ApJS, in press) made a 197-level calculation, using the R-matrix approach with the intermediate coupling frame transformation method. Excitation to n=4 is also included plus some correlation
- Before discussing their results examine the near threshold resonances in more detail
• Results of two new R-matrix Breit-Pauli calculations using the same target wave functions as Storey, Mason & Saraph (1996)

• The large value of the thermally averaged collision strength at $\approx 10^4 \text{K}$ is due to the near threshold group of resonances
Analysis shows that the large resonance features are \( n=7 \) Rydberg states with relatively high angular momentum, attached to the tenth target level, which is \( 3s3p^2 \,^2P_{3/2} \)

<table>
<thead>
<tr>
<th>( J_\pi )</th>
<th>( nl )</th>
<th>Energy (eV)</th>
<th>( \nu_{10} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2^e )</td>
<td>7g</td>
<td>0.120</td>
<td>6.9820</td>
</tr>
<tr>
<td>( 3^e )</td>
<td>7g</td>
<td>0.032</td>
<td>6.9755</td>
</tr>
<tr>
<td></td>
<td>7g</td>
<td>0.134</td>
<td>6.9830</td>
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<tr>
<td></td>
<td>7g</td>
<td>0.236</td>
<td>6.9906</td>
</tr>
<tr>
<td>( 4^o )</td>
<td>7h</td>
<td>0.216</td>
<td>6.9891</td>
</tr>
<tr>
<td></td>
<td>7h</td>
<td>0.532</td>
<td>7.0126</td>
</tr>
<tr>
<td>( 4^e )</td>
<td>7g</td>
<td>0.235</td>
<td>6.9905</td>
</tr>
<tr>
<td></td>
<td>7i</td>
<td>0.341</td>
<td>6.9984</td>
</tr>
</tbody>
</table>

etc
• The key point is that states with \( l = 4, 5, 6 \) have effective quantum numbers very close to the integer value and almost exclusively with \( \nu_{10} < 7 \)

• We can expect that theory will position them very accurately relative to the relevant threshold

• This would not necessarily be so for low \( l \) states
• The two new large scale calculations referred to above both use theoretical target energies for the thresholds
• However, both calculations place the tenth level too high by about 0.04 Ryd or 0.5eV
• If we return to the updated Storey et al (1996) calculation but adjust the target energies to the experimentally known ones
• The 0.5eV downward correction to the $3s3p^{2}\,^{2}P_{3/2}$ threshold causes the whole $n = 7$ resonance group to fall below the $^{2}\!^{2}P_{3/2}^{0}$ level in the elastic scattering region.
• The thermally averaged collision strength falls to $\approx 0.7$ between $10^4 - 10^5K$.
Latest theory compared to experiment

- Measurements of the near threshold cross-section have recently been made by Hossain *et al* (Phys. Rev. A, 75, 022709, 2007)
Cross-section can be converted to collision strength approximately by dividing by 2.2 at the position of the peak.
Thermally averaged collision strengths

Summary

- Large scale R-matrix calculations using **theoretical** thresholds broadly agree with experiment for the Fe xiv $^2\text{P}^0_{1/2} - ^2\text{P}^0_{3/2}$ near threshold collision strength
- Using **experimental** threshold energies pushes the near threshold resonances below the $^2\text{P}^0_{3/2}$ level in marked disagreement with experiment
- The resulting thermally averaged collision strengths are a better match to the Seyfert models
- At present theory, observation and experiment cannot be reconciled
- Empirical uncertainty in theory - Storey, Mason & Saraph, 30% at $10^6\text{K}$, factor 10 at $10^4\text{K}$. Latest theory results agree at $10^6\text{K}$, factor five at $10^4\text{K}$
- A rather extreme case but with the best current theory **ab initio** thresholds (and resonance series) are uncertain at the 0.5eV level